TT 72: Low-Dimensional Systems: Poster Session

Time: Wednesday 15:00–18:00 Location: Poster B

TT 72.1 Wed 15:00 Poster B

Detecting classical phase transitions using higher order Renyi entropies — •Wilfried Michel, Peter Broecker, and Simon Trebst — University of Cologne, Germany

Entanglement entropies have become a well-established tool to describe and characterize the ground-state properties of quantum many-body systems. In particular, these entropies allow to positively identify topological order and to detect and classify phase transitions even in the absence of any order parameter.

Though classical systems show no entanglement, one can define similar subsystem entropies that much like in the quantum case provide a generic way to study many features of classical systems. Here we consider so-called Renyi entropies, which are indexed by a positive integer $n \geq 1$ where the limiting case of $n = 1$ is the von-Neumann entropy.

In this contribution, we show how to efficiently calculate a series of higher-order Renyi entropies to high accuracy. This series of higher-order Renyi entropies is then used to calculate the classical analogue of the so-called entanglement spectrum using a maximum entropy approach. We illustrate this procedure for a number of classical models, including Ising and dimer models.

TT 72.2 Wed 15:00 Poster B

Phases and phase transitions in a rotated Kitaev model — •Eoin Quinn, Roderich Moessner, and Subhro Bhattacharjee — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

We investigate a variant of Kitaev's honeycomb model which also realises an exactly solvable quantum spin liquid, and analyse an extended phase diagram that takes into account Heisenberg perturbations and a magnetic field. The system has essential differences from the original construction of Kitaev, with interesting consequences appearing already in the exact solution. In an appropriate limit, the model reduces to a toric code model on a Kagome lattice. The effect of the Heisenberg interactions are examined using a combination of analytical and numerical approaches, and in the toric code limit we find a continuous quantum phase transition between the quantum spin liquid and a magnetically ordered phase which belongs to the 3D-XYxZ2 universality class.

TT 72.3 Wed 15:00 Poster B

Interplay of multiple charge-density-waves and superconductivity in $DyTe_3$ at high pressures — •Diego A. Zocco[1,4], Andreas Kapuvari[1], Aaron Sauer[1], Frank Weber[1], Parisiadis Paraskevas[2], Gaston Garbarino[2], Ian Fisher[3], James Hamlin[4], and Brian Maple[4] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]European Synchrotron Radiation Facility, F-38043 Grenoble Cedex, France — [3]Department of Applied Physics, Stanford University, CA 94305, USA — [4]Department of Physics, University of California, San Diego, CA 92093, USA

$DyTe_3$ is a quasi-two-dimensional system in which two successive incommensurate charge-density-wave (CDW) states appear upon cooling at ambient pressure ($T_{CDW,1} = 306\,K$, $T_{CDW,2} = 49\,K$). The suppression with pressure of the CDW order is followed by the emergence of superconductivity above 1 GPa and below 1.5 K, as shown by our measurements of electrical resistivity and ac-susceptibility. X-ray diffraction (XRD) experiments under pressure indicate that the lower CDW state merges with the upper one at an intermediate pressure, suggesting that the double-CDW state could be accessed directly below a single $T_{CDW}(P)$ line. The phase diagram obtained from XRD is compared with the results of our recent electrical resistivity experiments.

TT 72.4 Wed 15:00 Poster B

X-ray diffraction studies of charge-density-wave formation in $DyTe_3$ — •Aaron Sauer[1], Diego A. Zocco[1], Andreas Kapuvari[1], Frank Weber[1], Paula Giraldo-Gallo[2], Hsueh-Hui Kuo[2], and Ian R. Fisher[2] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany. — [2]Department of Applied Physics, Stanford University, CA 94305, USA.

We report measurements of the order parameters of the charge-density-wave (CDW) states in $DyTe_3$ using 4-circle x-ray diffraction from 5 K to 400 K. Rare-earth tritellurides (RTe_3) are quasi-two-dimensional materials in which CDW order develops in the Te-Te layers. The weakly-distorted tetragonal lattice allows, for the heavier rare-earth compounds, the formation of a second CDW state at lower temperatures, orthogonal to the first one. For example, $DyTe_3$ orders below $T_{CDW,1} = 306\,K$ and $T_{CDW,2} = 49$ K. The CDW order parameter is determined from the temperature evolution of the integrated intensity of the superstructure peaks. In particular, we studied how the upper CDW state is affected below $T_{CDW,2}$.

TT 72.5 Wed 15:00 Poster B

Superconductivity at the interface of $SrTiO_3$ and amorphous Al_2O_3 — •Roland Schäfer[1], Dirk Fuchs[1], Ahmed Sleem[1], Rudolf Schneider[1], Richard Thelen[2], and Hilbert von Löhneysen[1,3] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Mikrostrukturtechnik, 76021 Karlsruhe — [3]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe

We investigate the two-dimensional (2D) electron gas forming at the interface of TiO_2 terminated $SrTiO_3$ and amorphous Al_2O_3. The resistance drops on cooling from room temperature down to 200 mK in an usual way by a factor of up to 250. Below 200 mK the system becomes superconducting. We investigate the superconducting phase transition by analyzing voltage vs. current (V/I) characteristics as a function of temperature and magnetic field. The I/V characteristics show a power law scaling $V \propto I^{\alpha}$ at low bias with a temperature dependent exponent α which is close to 1 at high temperatures rises to 3 at around $T \approx 160$ mK and rapidly ascents on further lowering the temperature. This behaviour is typical for a Berezinskii-Kosterlitz-Thouless transistion found in 2D superconductive layers.

TT 72.6 Wed 15:00 Poster B

Superconducting fluctuations in systems with Rashba-spin-orbit coupling — •Stefan Beyl[1], Peter P. Orth[2], Mathias Scheurer[2], and Jörg Schmalian[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Deutschland

We investigate the BEC-BCS crossover in a two-dimensional system with Rashba-spin-orbit coupling. To include the effects of phase and amplitude fluctuations of the superconducting order parameter we perform a loop expansion of the effective field theory. We analyze in particular the probability of a low density superconducting quantum phase transition. The theory is relevant to $LaAlO_3/SrTiO_3$ interfaces and two-dimensional cold atom systems with synthetic gauge fields.

TT 72.7 Wed 15:00 Poster B

Oxygen stoichiometry of $LaTiO_3$ thin films studied by *in-situ* photoemission — •Philipp Scheiderer, Alex Goessmann, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

As in the famous oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a two dimensional electron system is found at the interface between the strongly correlated Mott insulator $LaTi^{3+}O_3$ and the band insulator STO. The stabilization of $LaTi^{3+}O_3$ requires strong reducing growth conditions since the thermodynamically stable bulk phase is the oxygen rich $La_2Ti^{4+}{}_2O_7$. Therefore, we have systematically studied the impact of the oxygen background atmosphere on $LaTi^{3+}O_3$ thin film growth by PLD. Reflection high-energy diffraction intensity oscillations of the specular spot indicate a layer by layer growth mode for thin films, which merges into the formation of islands for thicker films. *In-situ* photoemission measurements enables us to determine the oxidation state of Ti indicating excess or lack of oxygen present in the prepared samples. Our experiments show that even for films grown in vacuum, strong oxygen excess is present probably due to oxygen outdiffusion from the STO substrate. We find that an LAO buffer layer serves as an effective barrier for this process. The spectral weight of the lower Hubbard band, being a characteristic feature for the Mott insulating phase, is found to scale inversely with the amount of excess oxygen.

TT 72.8 Wed 15:00 Poster B

Resonant photoelectron spectroscopy of γ-Al_2O_3/$SrTiO_3$ heterostructures — •Philipp Schütz[1], Florian Pfaff[1], Michael Zapf[1], Judith Gabel[1], Lenart Dudy[1], Götz Berner[1], Yunzhong Chen[2], Nini Pryds[2], Victor Rogalev[3], Vladimir Strocov[3], Christoph Schlüter[4], Tien-Lin Lee[4], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Würzburg, Germany — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Risø Campus, Denmark — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [4]Diamond Light Source Ltd., Didcot, United Kingdom

The spinel/perovskite heterointerface between the band insulators γ-Al_2O_3 and $SrTiO_3$ hosts a two-dimensional electron system (2DES) with exceptionally high electron mobility. Soft x-ray resonant photoelectron spectroscopy at the Ti L absorption edge is used to probe the Ti 3d derived interface states. Marked differences in the resonance behavior are found for the $SrTiO_3$ valence band and the different interface states, which are observed in the band gap of $SrTiO_3$. A comparison to x-ray absorption spectra of Ti $3d^0$ and Ti $3d^1$ systems reveals the presence of different types of electronic states with Ti 3d character, i.e., oxygen vacancy induced, trapped in-gap states and itinerant states contributing to the 2DES. Furthermore, exposure to low doses of oxygen during irradiation allows for the controlled and reversible manipulation of the interfacial electronic structure, i.e., the in-gap state intensity and the valence band offset between $SrTiO_3$ and γ-Al_2O_3.

TT 72.9 Wed 15:00 Poster B

Synthesis and electrical transport properties of the $LaVO_3$/$SrTiO_3$ interface — •Richard Hentrich[1], Jens Hänisch[1,2], Ludwig Schultz[1], and Ruben Hühne[1] — [1]IFW Dresden, Germany — [2]ITEP, Karlsruhe Institute of Technology (KIT), Germany

We have investigated the two dimensional electron gas at the interface of band gap insulator $SrTiO_3$ and mott insulator $LaVO_3$ in comparison to the well-known, purely band insulating $LaAlO_3$/$SrTiO_3$ system. Thin films of $LaVO_3$ were grown epitaxially on TiO_2 terminated $SrTiO_3$ single crystal substrates using RHEED-monitored pulsed laser deposition. Optimal process parameters for layer-by-layer growth were found resulting in the growth of atomically smooth films of well-defined thickness. Electrical transport measurements revealed an insulator-metal transition at a film thickness of six unit cells, which is different to previously reported values. Conducting samples showed metallic behavior in a wide temperature range, with their conductivity showing little to no dependence on layer thickness. This led to the conclusion of the metallic behavior being a merely interface driven effect.

TT 72.10 Wed 15:00 Poster B

Torque magnetometry on two-dimensional electron systems at MgZnO/ZnO interfaces — •Schorsch Michael Sauther[1], Stephan Albert[1], Matthias Brasse[1], Joseph Falson[2], Yusuke Kozuka[2], Atsushi Tsukasaki[3], Marc Andreas Wilde[1], Masashi Kawasaki[2,4], and Dirk Grundler[1] — [1]Phys.-Dep. E10, TU München — [2]Dep. of App. Phys. and QPEC, University of Tokyo — [3]IMR, Tohoku University and JST PRESTO — [4]RIKEN CEMS

Two-dimensional electron systems (2DESs) in oxide heterostructures have created great interest in the recent years. We study the magnetization M of MgZnO/ZnO heterostructures with 2DESs of small carrier density and high mobility at low temperatures and in high magnetic fields B. We report the de Haas-van Alphen (dHvA) effect, non-equilibrium currents (NECs) and unexpected overshoots in $M(B)$. An investigation of the temperature dependence of the dHvA amplitude allows us to determine the effective masses of the electron systems. We find enhanced effective masses and enhanced dHvA amplitudes. The NEC signals are analyzed regarding their dependence on temperature and magnetic field sweep rate. We explain the unexpected overshoots of the dHvA amplitude by means of the magnetic thaw-down effect which allows us to identify the type and density of charged impurities in the heterostructures. In addition, we report a hysteretic feature in the dHvA effect that we discuss in the framework of quantum Hall ferromagnetism. The work is supported by the DFG via TRR80 and Grant-in-Aids for Scientific Research (S) No. 24226002 from MEXT, Japan, as well as by the Murata Science Foundation.

TT 72.11 Wed 15:00 Poster B

Temperature dependent optical spectra of magnetic excitations of a 4-leg ladder — •Ignacio Vergara[1], Kris Cöster[2], Luis Fels[1], Martin Valldor[1,3], Stefan Wessel[4], Kai Phillip Schimdt[2], and Markus Grüninger[1] — [1]II. Physicalisches Institut, Universität zu Köln — [2]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund — [3]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University

In low-dimensional spin-1/2 cuprates, optical spectroscopy is a powerful tool for the study of magnetic excitations with total spin S=0, e.g., bimagnon-plus-phonon absorption. The simultaneous excitation of a symmetry-breaking phonon allows us to study the magnetic excitations at high energies ($\sim$ 0.1 - 1 eV) throughout the entire Brillouin zone, because the phonon takes care of momentum conservation. The line shape of the optical conductivity provides important information on the kinetics and on the interactions of the magnetic excitations.

Through n-leg S=1/2 cuprate ladders, one can explore the dimensional crossover between 1D and 2D systems. The magnetism of n-leg ladders is of particular interest due the possible relevance for high T_c superconductivity. We present temperature-dependent optical conductivity data of the 4-leg ladder $La_2Cu_2O_5$. We report on a pronounced two-triplon resonance and compare the results with optical spectra of a 2-leg ladder compound and theory (CUT, QMC). Calculations for open and closed boundary conditions give insight on the character of the observed excitations.

TT 72.12 Wed 15:00 Poster B

Mott metal-insulator transition induced by utilizing a glass-like structural ordering in low-dimensional molecular conductors — •Benedikt Hartmann[1], Jens Müller[1], and Takahiko Sasaki[2] — [1]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt (M), Germany — [2]Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan

We utilize a glass-like structural transition in order to induce a Mott metal-insulator transition in the quasi-two-dimensional organic charge-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br. In this material, the terminal ethylene groups of the BEDT-TTF molecules can adopt two different structural orientations within the crystal structure, namely eclipsed (E) and staggered (S). When cooling through the glass transition at $T_g \simeq 75$ K, a small fraction that depends on the cooling rate remains frozen in the S configuration. We demonstrate that, when thermally coupled to a low-temperature heat bath, a pulsed heating current through the sample causes a very fast relaxation with cooling rates at T_g of order several 1000 K/min. The freezing of the structural orientation causes a decrease of the electronic bandwidth W with increasing cooling rate, and hence a Mott metal-insulator transition as the system crosses the critical ratio $(W/U)_c$ of bandwidth W to on-site Coulomb repulsion U. Due to the glassy character of the transition, the effect is persistent below T_g and can be reversibly repeated by melting the frozen configuration upon warming above T_g. A simple model allows for an estimate of the energy difference between the E and S state as well as the cooling rate dependent difference in population.

TT 72.13 Wed 15:00 Poster B

Thermal expansion and magnetostriction measurements of the mixed systems $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$) — •Satya Krishna Thallapaka, Ulrich Tutsch, Lars Postulka, Bernd Wolf, Michael Lang, Natalia van Well, Franz Ritter, and Cornelius Krellner — Physics Institute, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany

The mixed systems $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$), including the two well-known end members Cs_2CuCl_4 and Cs_2CuBr_4, are classified as quasi-two-dimensional quantum antiferromagnets with different degrees of magnetic frustration. Due to a site-selective substitution of the halide atoms two distinct critical concentrations (x = 1 and x = 2) had been identified [1]. Especially the $Cs_2CuCl_2Br_2$ compound exhibits the potential to be the system with the highest degree of frustration within this series. We present low-temperature thermal expansion measurements down to 40 mK and magnetostriction experiments up to 14 T on the $Cs_2CuCl_2Br_2$ compound. While specific heat measurements reveal indications for magnetic order around 90 mK, no clear signatures were found in thermal expansion studies along the b axis. Here an in-T linear contribution was observed indicating a 1D character of the magnetic excitations. For fields above 5 T one finds a clear deviation from this linearity. These results are discussed with specific heat data and also compared with the thermodynamic properties of the pure Cs_2CuCl_4 compound.

[1] P. T. Cong et al., Phys. Rev. **B** 83, 064425 (2011)

TT 72.14 Wed 15:00 Poster B

Field-induced ordered phases in coupled spin-dimer systems — •L. Postulka[1], B. Wolf[1], U. Tutsch[1], M. Baumgarten[2], Y. Borozdina[2], D. Strassel[3], S. Eggert[3], and M. Lang[1] — [1]Physics Institute, Goethe-University, SFB/TR 49, D-60438 Frankfurt (M) — [2]Max-Planck-Institute for Polymer Research, SFB/TR 49, D-55128 Mainz — [3]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern

Materials built of antiferromagnetically-coupled S=1/2 dimers, allow to study finite-temperature critical phenomena under well-controlled conditions. Examples are the Bose-Einstein-condensation of magnons in 3D systems and Luttinger-liquid behaviour in 1D. In pure 2D materials one expects so-called topological order associated with the binding of vortices with opposite circulation as suggested by Berezinskii, Kosterlitz and Thouless. We present susceptibility data down to 27 mK of a newly synthesised S=1/2 spin dimer systems consisting of stable organic biradicals. The crystal structure suggests a 2D arrangement of the coupled dimers. We observe a field-induced ordered state characterized by a rounded double-peak structure. To obtain detailed information about the nature of the field-induced ordered phase we measured the temperature dependence of the susceptibility at the critical fields. These results are compared with quantum Monte Carlo simulations and measurements on a metal-organic compound, composed of layers of S=1/2 dimers, which lacks long-range 3D magnetic order down to at least 27 mK, but instead shows distinct 2D behaviour in its magnetic properties[1].

[1] Tutsch *et al.*, Nat. Commun. 5, 5169 (2014)

TT 72.15 Wed 15:00 Poster B

Field and angle dependent magnetoresistance oscillations in the normal and antiferromagnetic states of κ-(BETS)$_2$FeX$_4$ (X = Cl, Br) — •Michael Kunz[1], Ludwig Schaidhammer[1], Werner Biberacher[1], Natasha D. Kushch[2], and Mark V. Kartsovnik[1] — [1]Walther- Meißner-Institut, Garching, Germany — [2]Institute of Problems of Chemical Physics, Chernogolovka, Russia

The bifunctional materials κ-(BETS)$_2$FeX$_4$ (X = Cl, Br) are layered organic metals exhibiting both metallic and superconducting behaviour while carrying localised magnetic moments. These compounds show an anitferromagnetic ground state with Néel temperatures T_N of 0.46 K and 2.5 K respectively, while the electron system remains metallic even below T_N. Studies of field and angular sweeps of the interlayer magnetoresistance for different field directions revealed different kinds of angular-magnetoresistance-oscillations (AMRO) as well as Shubnikov-de Haas (SdH) oscillations. The experimental data will be discussed in the context of the Fermi surface properties and their response to the antiferromagnetic ordering.

TT 72.16 Wed 15:00 Poster B

Hints for a pressure-induced insulator-to-metal transition in low-dimensional CuNCN — •Estaline Amitha Francis[1], H. Rosner[2], and C. A. Kuntscher[1] — [1]Experimentalphysik 2, Universität Augsburg, D-86135 Augsburg, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Copper oxide compounds show fascinating properties such as high temperature superconductivity, cooperative Jahn-Teller effect, spin-Peierls magnetic, and cooperative magnetic states. Copper carbodiimide (CuNCN) is the nitrogen-based analog of cupric oxide, where the oxygen anion O^{2-} is replaced with the isolobal carboiimide NCN^{2-}, resulting in a distorted octahedral with first-order Jahn-Teller effect. Infrared high-pressure measurements on CuNCN were performed over the frequency range 500–6000 cm^{-1} to probe the insulator-to-metal transition. The infrared phonons of CuNCN at 595 and 696 cm^{-1} show significant pressure-dependent softening. The phonon mode at 595 cm^{-1} shows a two-fold splitting at 5 GPa (P_{c1}) and further splittings around 11 GPa (P_{c2}). The absorption edge is observed around 1200 cm^{-1} for 0.3 GPa and shows a strong red shift above P_{c2}. Furthermore, we observe a smearing out of the phonon spectra above P_{c2}. The changes in the absorption edge and the smearing out of phonons are indications for a pressure-induced insulator-to-metal transition in CuNCN.

TT 72.17 Wed 15:00 Poster B

Ferromagnetic domains due to a double exchange mechanism — •Matthias Peschke and Michael Potthoff — I. Institut für Theoretische Physik, Hamburg, Deutschland

The doped one-dimensional Kondo lattice is known to be ferromagnetic for sufficiently strong exchange coupling J. Ferromagnetism is caused by a double-exchange mechanism, i.e., electrons gain kinetic energy for ferromagnetically aligned local moments. For one-dimensional ring structures, however, this seemingly clear situation becomes much more complicated. Employing Krylov-space methods for finite Kondo lattices at strong J, we find that a singlet ground state is favored in some cases depending on the electron number and the boundary conditions. We argue that, locally, the double exchange leads to ferromagnetic alignment but globally the local moments may form a domain structure to prevent ring processes of the electrons, which are unfavorable due to the Fermi statistics or due to the boundary conditions.

TT 72.18 Wed 15:00 Poster B

Calculation of correlation functions of the Heisenberg chain by means of a hidden fermionic structure — •Raphael Kleinemühl and Frank Göhmann — Bergische Universität Wuppertal

We study short-distance correlation functions of the homogeneous XXZ chain by means of a hidden fermionic structure discovered by Boos et.al. Using computer algebra we explicitly construct the fermionic operators needed in this approach. They act on the space of quasilocal operators on the XXZ chain. For small n we express products of local operators, like $\sigma_1^z\sigma_n^z$, in terms of the fermionic basis, i.e. by acting with creation operators on a certain vacuum state. Short distance correlation functions appear in various physical applications as e.g. in the calculation of moments of ESR spectral lines. Apart from that it is our goal to extend the approach in such a way that a calculation of correlation functions of large distances becomes possible.

TT 72.19 Wed 15:00 Poster B

Hardware-independent Parallelization of Matrix Product State Codes Using SciPAL — •Thomas Köhler[1], Johannes Hagemann[2], Salvatore R. Manmana[1], and Stephan C. Kramer[3] — [1]Institut f. Theoretische Physik, Universität Göttingen — [2]Institut f. Röntgenphysik, Universität Göttingen — [3]Max-Planck-Institut f. biophysikalische Chemie, Göttingen

The physical properties of low-dimensional, strongly-correlated quantum systems, as described by Hubbard-like or Heisenberg models, can efficiently be accessed by matrix product state (MPS) and density-matrix renormalization group (DMRG) methods. The key to an efficient MPS code is the optimization of the evaluation of concatenated matrix-matrix products for building the multi-particle states and an efficient compression of single-particle states by truncated singular value decompositions. Based on SciPAL's [1] expression templates for BLAS operations we have designed a domain-specific embedded language for computing the properties of MPS. Because SciPAL's expression templates are hardware-independent we can provide an objective comparison of the performance of CPU- or GPU-based computations and hybrid forms thereof.

[1] SciPAL: Expression Templates and Composition Closure Objects for High Performance Computational Physics with CUDA and OpenMP, S. C. Kramer and J. Hagemann, ACM TOPC (to appear).

TT 72.20 Wed 15:00 Poster B

Electronic Instabilities of the AA-Honeycomb Bilayer — •David Sánchez de la Peña[1], Michael Scherer[2], and Carsten Honerkamp[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany and JARA Fundamentals of Future Information Technologies — [2]Institute for Theoretical Physics, University of Heidelberg, D-69120 Heidelberg, Germany

We use a functional renormalization group approach to study the instabilities due to electron-electron interactions in a bilayer honeycomb lattice model with AA stacking, as it might be relevant for layered graphene with this structure. Starting with a tight-binding description for the four π-bands, modes of the dispersion are integrated out by successively lowering an infrared cutoff. For a given set of short-ranged interactions, the method allows for an unbiased investigation of the competing instabilities arising in the effective low-energy theory, and for the determination of the leading tendencies. The antiferromagnetic spin-density wave is an expected instability for dominant local repulsion among the electrons, but for nonlocal interaction terms also other instabilities occur. The resulting phase diagrams depending on the model parameters are presented. We compare our results to single-layer graphene and the more common AB-stacked bilayer, both qualitatively and quantitatively. Current prospects for the analysis of graphene systems using some of the latest developments in renormal-

ization group methods are also discussed.

TT 72.21 Wed 15:00 Poster B

Strongly Degenerate Fermions in 2D Quantum Dots at Finite Temperatures - Configuration Path Integral Monte Carlo — •Simon Groth, Tim Schoof, and Michael Bonitz — Institut for Theoretical and Astrophysics, Christian Albrechts Universität Kiel, Germany

Based on first principles, the configuration PIMC approach (CPIMC) allows for the exact computation of thermodynamic properties of strongly degenerate fermionic many-body systems with arbitrary pair-interaction [1,2]. Due to the fermion sign problem, this regime is not accessible with (standard) PIMC methods. Here, a Worm algorithm within the CPIMC formalism is presented which, in addition to standard thermodynamic observables, is capable of providing exact results for imaginary time correlation functions, i.e., in particular for the Matsubara Green function. The method is tested for a two-dimensional system of spin polarized, Coulomb interacting fermions in a harmonic trap. Further, sampling only paths from a subspace of the whole configuration space (Restricted CPIMC), the sign problem can be circumvented. The introduced systematic error vanishes with increasing degeneracy.

[1] T. Schoof, M. Bonitz, A. Filinov, D. Hochstuhl, and J. Dufty, Contrib. Plasma Phys. **51**, 687 (2011).

[2] T. Schoof, S. Groth and M. Bonitz, Introduction to Configuration Path Integral Monte Carlo, Chapter in: Complex Plasmas: Scientific Challenges and Technological Opportunities edited by M. Bonitz, K. Becker, J. Lopez and H. Thomsen (Springer 2014).