TT 47: Poster Session Correlated Electrons 2

Time: Wednesday 15:00–19:00 Location: P2/3OG

TT 47.1 Wed 15:00 P2/3OG

DMRG study of a Kagome strip with two types of site spins — •Felix Liedeker[1], Nedko Ivanov[1,2], and Jürgen Schnack[1] — [1]Universität Bielefeld, Fakultät für Physik — [2]Institute of Solid State Physics, Bulgarian Academy of Sciences

We study the quantum phase diagram and the low-lying excited states of a Heisenberg kagome strip containing two types of site spins and different exchange constants for the nearest-neighbor exchange bonds by means of the density matrix renormalization group (DMRG). Geometrically, this system is a cut out from the kagome lattice, so that a cluster of five spins repeats along the chain. In particular we study non-trivial phases apart from the standard ferromagnetic and ferrimagnetic phases.

TT 47.2 Wed 15:00 P2/3OG

Properties of effective potentials obtained within the Localisation Landscape Theory of random potentials — •Sebastian Luhn and Erich Runge — Technische Universität Ilmenau, Institut für Physik, 98693 Ilmenau

Anderson Localisation is the leading paradigm for localisation in random potentials, e.g. due to interface roughness and alloy disorder in semiconductor heterostructures. The so-called Localisation Landscape Theory of S. Mayboroda et al. maps disordered potentials to a family of much smoother "effective potentials", whose minima are likely candidates for localized states. We study these effective potentials for 1D Gaussian random distributed atom chains via numerical simulations and approximate analytical expressions. In particular we compare the distributions of extrema and the spatial correlation of the effective Potential to the properties of the original potential.

TT 47.3 Wed 15:00 P2/3OG

RPA as exact high-density limit of 1D correlated electrons — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[5] — [1]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics - UFRN, Campus Universitário Lagoa nova, 59078-970 Natal, Brazil — [3]Department of Physics, Dr. B.R. Ambedkar NationalInstitute of Technology, Jalandhar (Punjab) - 144 011, India — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum if the relation between Fermi energy and Fermi momentum is $\epsilon_{\rm f} \sim p_{\rm f}^{\beta}$ and the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d < \beta + \alpha$ specifies systems where RPA is exact in the high-density limit. The one-dimensional structure factor is calculated analytically and the ground-state energy is presented exactly in the high-density and Coulomb limit. The proposed high-density expansion agrees with diffusive Monte Carlo simulations which we performed for this purpose.

[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] arXiv:1909.09331

TT 47.4 Wed 15:00 P2/3OG

Thermal expansion and magnetostriction studies on $CoTiO_3$ — •Marco Hoffmann[1], Kaustav Dey[1], Sven Spachmann[1], Rabindranath Bag[2], Surjeet Singh[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]IISER Pune, Maharashtra, India

The $S = 3/2$ compound $CoTiO_3$ crystallizes in the ilmenite-type structure which belongs to the R-3 space group. In particular, it features a strong magnetoelectric coupling. Recent discovery of Dirac magnons [1] in this compound motivates further research on the interplay of electronic, magnetic and structural degrees of freedom. We have grown high-quality single crystals by means of the optical floating-zone method and have studied magnetisation, magnetostriction, thermal expansion and specific heat of $CoTiO_3$. Pronounced anomalies in the thermal expansion coefficients at the phase transitions evidence strong magnetoelastic coupling. The magnetic phase diagram evidences a spin-reoriented phase at low magnetic fields indicating small anisotropy within the *ab*-plane. Grüneisen scaling reveals the relevant energy scales of the ordering phenomena and the structural changes at the phase boundaries are discussed.

[1] Bo Yuan et al., arXiv:cond-mat/1907.02061v1

TT 47.5 Wed 15:00 P2/3OG

Strain engineering of the Mott material $LaTiO_3$ — •Berengar Leikert[1], Julia Küspert[1], Martin Stübinger[1], Matthias Schmitt[1], Judith Gabel[2], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg — [2]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE

3d transition metal oxides exhibit fascinating phenomena - absent in conventional semiconductors - like Mott insulating behaviour due to pronounced electron-electron interactions. The field of Mottronics dreams of harnessing the phase transition between the correlated metal and the Mott insulating phase of such strongly correlated materials for novel electronic devices.

We have recently demonstrated that the prototypical Mott insulator $LaTiO_3$ can undergo the band filling controlled Mott transition if it is chemically p-doped by excess oxygen during thin film growth by pulsed laser deposition [1]. Here we report on the influence of epitaxial strain. By using different substrates ($GdScO_3$, $DyScO_3$, $LaAlO_3$) we should be able to tune $LaTiO_3$ in the generic phase diagram (correlation strength versus band filling) from the Mott insulating phase towards the correlated metal phase [2]. Our goal is, exploiting strain and doping, to find an optimal spot in the phase diagram close to the boundary of the phase transition, where one might be able to trigger the phase transition with moderate electric fields.

[1] Scheiderer et al., Adv. Mater. 30, 1706708 (2018)
[2] Dymkowski et al. Phys. Rev. B 89, 161109 (2014)

TT 47.6 Wed 15:00 P2/3OG

Dielectric and Fluctuation (Noise) Spectroscopy as Complements Tools to Study Slow Dynamics in Electronic Systems with Frustration — •Giuseppe Cantarella, Merlin Mitschek, Benjamin Kammerbauer, Tatjana Thomas, and Jens Müller — Institute of Physics, Goethe University, Frankfurt (Main), Germany

The fluctuation-dissipation-theorem (FDT) quantifies the relation between the response of a system to external perturbations and its fluctuations at thermal equilibrium. In general the FDT connects the noise power spectral density (PSD) of a system with the dissipative part of susceptibility, χ''. As a consequence, in dielectric system like e.g. glasses, one can measure boths sides of the FDT equation and independently check the validity of the FDT [1]. Our aim is to explore a connection between the dielectric properties of a molecular Mott insulator and the conductance noise PSD, which often shoes a $1/f$ - type behaviour. As a test system, we chose the spin-liquid [2] candidate κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$, which is a dimer Mott insulator on a frustrated triangular lattice that exhibits anomalous dielectric relaxations which resemble that of relaxor ferroelectric materials with quantum electric dipoles. In this work, we present first results of complementary dielectric susceptibility and current noise measurements.

[1] Phys. Rev. Lett. **107**, 095701 (2011) [2] Phys. Rev. B **82**, 125119

TT 47.7 Wed 15:00 P2/3OG

Drastic change of the charge carrier dynamics at the Mott metal-insulator transition in κ-$(BETS)_2Mn[N(CN)_2]_3$ — •Yassine Agarmani[1], Tatjana Thomas[1], Mark Kartsovnik[2], Nataliya Kushch[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaft, Germany — [3]Institute of Problems of Chemical Physics, Russian Academy of Sciences, Russia

The quasi-two-dimensional organic conductor κ-$(BETS)_2Mn[N(CN)_2]_3$ combines strong electronic correlations with magnetic properties dominated by the presence of magnetic Mn^{2+} ions in the insulating polymeric anion layers. The system undergoes a superstructure transition near 102 K, presumably of structural origin, and a metal-insulator transition at $T_{\rm MI} \sim 30$ K likely associated with a Mott instability [1,2]. In order to investigate the dynamical properties of the charge carriers, fluctuation (noise) spectroscopy has proven to be a successful

method by measuring the time-dependent fluctuations of a sample's resistance [3]. In this compound the normalized noise power spectral density shows a broad maximum at $\sim 100\,\mathrm{K}$ and a dramatic increase below T_{MI}. The increase is accompanied by non-Gaussian fluctuations indicated by time-dependent noise spectra. In contrast, above T_{MI} there is a good agreement with a simple model assuming independent fluctuators allowing to determine characteristic energies. We discuss our results in light of the possibilities of electronic ferroelectricity, recently observed in a number of dimer-Mott insulators.
[1] JACS 130, 7238 [2] PRB 82, 155123 [3] Crystals 8, 166

TT 47.8 Wed 15:00 P2/3OG

Magnetic phase diagram of Li_2FeSiO_4 — •Ahmed ElGhandour[1], Martin Jonak[1], Waldemar Hergett[1], Sven Spachmann[1], Mahmoud Abdel-Hafiez[1,2], Johannes Werner[1], Sven Sauerland[1], Nadejda Bouldi[3], Maurits Haverkort[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Faculty of Science, Physics Department, Fayoum University, Egypt — [3]Institut für Theoretische Physik, Heidelberg University, Germany

Li_2FeSiO_4 single crystals of *Pmnb*-structure exhibit tetrahedrally coordinated Fe^{2+}-ions in high-spin configuration and quasi-2D magnetic substructures. The anisotropy gap $\Delta = 2.9$ meV implies significant anisotropy as compared to the antiferromagnetic dominant in-plane couplings along the crystallographic *a*- and *c*-directions, i.e., 1.0 and 3.6 meV, respectively. Notably, long-range AFM order evolving at $T_{\mathrm{N}} = 17$ K is nearly completely suppressed by magnetic fields of 16 T. While, at higher magnetic fields additional phases appear which extend to 35 T and around 15 K. In addition to the unusual magnetic phase diagram, short-range correlations at least up to $T \approx 110$ K are discussed with respect to short-range magnetic order and low-energy orbital excitations within the low-lying e_g-orbitals.

TT 47.9 Wed 15:00 P2/3OG

Ultrafast dynamics in transition-metal dichalocogenide $IrTe_2$ — •Amrit R Pokharel[1], Meng Yang[2], You Guo Shi[2], Tao Dong[1], and Jure Demsar[1] — [1]Uni Mainz, Germany — [2]Institute of physics, CAS, China

Layered transition-metal dichalocogenide $IrTe_2$ undergoes a structural phase transition to a(1/8, 0, 1/8) modulated state at T_c 280 K, followed by a transition to a(1/5, 0, 1/5) lattice modulated phase around 170 K. The low temperature modulated phase is further accompanied by the emergence of superconductivity below 2 K. Upon warming, the low temperature (1/5, 0, 1/5) lattice modulated phase persist up to T_c 280 K without entering into the (1/8, 0, 1/8) modulated state. The structural phase transitions are accompanied by sharp jumps in resistivity, indicating a complex electronic modulation entangled with structural phase transition. Despite the extensive studies, origins of the structural phase transitions and possible non-thermal light induced phase transitions remain elusive. We study the carrier relaxation dynamics and collective modes in different phases of $IrTe_2$ utilizing time-resolved pump-probe spectroscopy. Upon cooling below 280 K we observe the emergence of A1g modes at 1.28 THz and 2.17 THz. Upon further cooling through 170 K the 2.17 THz mode is dramatically reduced and new modes appear near 2.52 THz. On warming up from liquid-He temperatures the low frequency phonon modes remain unchanged up to 280 K, without entering the intermediate phase. These observations suggest the coherent phonon spectroscopy to be a sensitive tool to probe the symmetry breaking phase transitions.

TT 47.10 Wed 15:00 P2/3OG

Theoretical study of designer Hubbard models — •David Mikhail and Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

There has been tremendous progress towards engineering of tuneable two-dimensional Hubbard models in Si:P systems using scanning tunnelling microscopy (STM). STM placement allows for localization of dopants with atomic-scale precision. Motivated by these recent experimental developments, we theoretically study low-dimensional phosphorus lattices in the framework of the Hubbard model. We numerically calculate local properties of the dopants like the local density of states as well as local correlations of spin and charge. These features are experimentally accessible through scanning tunnelling spectroscopy measurements. Additionally, we investigate electronic transport properties which can be measured in standard experiments. Atomically engineered nanostructures represent promising candidates for quantum many-body simulators of strongly correlated fermionic systems, which are known to exhibit exotic physics such as high-Tc superconductivity and topological phases. The discussed Si:P systems constitute a competitive alternative to cold atoms in optical lattices as for the former much lower temperature scales can be reached.

TT 47.11 Wed 15:00 P2/3OG

Electronic structure and dynamical properties of KO_2 — •Dorota Gotfryd[1,2], Olga Sikora[3], Andrzej Ptok[3], Andrzej M. Oles[2,4], Krzysztof Wohlfeld[1], and Przemyslaw Piekarz[3] — [1]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [2]Institute of Physics, Jagiellonian University, Lojasiewicza 11, PL-30348 Krakow, Poland — [3]Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342 Krakow, Poland — [4]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Here we investigate the possible mechanisms behind the insulating properties of the strongly correlated superoxide KO_2. The intermediate monoclinic C2/c phase with O_2 molecules rotated by about 20 deg from the high-temperature tetragonal structure reported in experiments is here examined by means of density functional theory and lattice dynamics. We identify a soft phonon leading to the new stable distorted phase of C2/c symmetry and analyse its structural properties. Comparison of the electronic structure of KO_2 in the tetragonal and monoclinic phases reveals the insulating mechanism in the monoclinic phase: while only the joint efforts of large on-site Coulomb and small spin-orbit interactions are able to open a small charge gap in the tetragonal phase, in the monoclinic phase perturbing GGA+U by the small spin-orbit coupling moves KO_2 from weak to strong Mott-insulator regime. This indicates an important role of the interplay between Coulomb and on-site spin-orbit interactions as well as pronounced lattice distortions in formation of the insulating phase.

TT 47.12 Wed 15:00 P2/3OG

LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Correlated Materials — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We present a computational study of *L*-edge resonant inelastic x-ray scattering (RIXS) in 3*d* transition-metal (TM) oxides: NiO; $RNiO_3$; Fe_2O_3; $SrCoO_3$, $LaCoO_3$ and $LiCoO_2$; $LaCuO_3$ and $NaCuO_2$ [1]. We apply exact diagonalization to a material specific Anderson impurity model with a by DMFT obtained hybridization function. In contrast to other available methods, this approach enables us to describe simultaneously localized (*d*-*d*) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. Our calculated results reproduce well the experimental data and RIXS can be used as a tool to study material-specific hybridization between x-ray excited TM ion and low-energy states.
[1] A. Hariki, M. Winder, and J. Kuneš, Phys. Rev. Lett. **121**, 126403 (2018)

TT 47.13 Wed 15:00 P2/3OG

Interplay of electronic structure, magnetic state, and lattice stability in iron oxides under extreme conditions — •Ivan Leonov — M.N. Mikheev Inst. of Metal Physics, Yekaterinburg, Russia — NUST 'MISiS', Moscow, Russia

The theoretical understanding of iron oxides is of fundamental importance for modeling the properties and evolution of the Earth's interior. Here, we employ the DFT+DMFT method to determine the electronic structure, magnetic state, and structural phase stability of paramagnetic hematite Fe_2O_3 and pyrite-type FeO_2. Our results reveal a complex interplay between electronic correlations and the lattice in these compounds under extreme conditions. In particular, in the vicinity of a pressure-induced Mott transition Fe_2O_3 exhibits a series of complex electronic, magnetic, and structural transformations, which are accompanied by a site-selective collapse of local magnetic moments and delocalization of the Fe 3*d* electrons. Our results for structural optimization of FeO_2 within DFT+DMFT show that FeO_2 is a metal and that the oxidation state of Fe is equal to nearly 3+. In contrast to the previous claims, we found no noticeable oxygen-oxygen bonding in FeO_2 to at least 180 GPa (no evidence for the O_2 dimerization), implying that the oxidation state of oxygen in pyrite-type FeO_2 is 1.5- due to the oxygen-to-iron negative charge transfer. Our calculations of the relative phase stability of FeO_2 and Fe_2O_3 reveal that FeO_2 is unstable below ∼40 GPa. In agreement with experiment, it is found to decompose into Fe_2O_3 with release of oxygen, suggesting the im-

portance of iron oxides in oxygen cycling between Earth's reservoirs.

TT 47.14 Wed 15:00 P2/3OG

Exploring quasi-molecular orbitals in iridates by cluster RIXS calculations — •Jan Attig[1], Maria Hermanns[2], and Markus Grüninger[3] — [1]Institut für Theoretische Physik, Universität zu Köln, Germany — [2]Stockholm University, Sweden — [3]II. Physikalisches Institut, Universität zu Köln, Germany

In recent years, the spin-orbit assisted Mott-insulating behavior of many iridate compounds has been established as a rich playground for quantum magnetism and novel phases of matter, since control in the compound structure allows to tune the subtle interplay of Hubbard interaction, spin-orbit coupling and hopping. In particular it has been shown that for Ir_2O_9 dimers in $Ba_3CeIr_2O_9$, the electronic structure consists of quasi-molecular orbitals on those dimers, which can be probed by observing a double-slit like interference pattern in resonant inelastic X-ray scattering (RIXS) [1].

Here, we present an approach that allows systematic investigation of quasi-molecular orbitals in various iridate compounds by calculation of the respective RIXS signatures from exact diagonalization (ED). We present ED calculations of the electronic structure on individual clusters of IrO_6 octahedra, as well as their RIXS spectrum. Our calculations are performed by an effective, numerical framework which is implemented on a dynamical level within the programming language Julia. This framework allows us to investigate sytems with adjustable geometry, varying number of IrO_6 octahedra, as well as different number of electrons within the system.

[1] A. W. Sleight, *Phys. C* **514**, Revelli et al., Science Advances 2019, 5: eaav4020

TT 47.15 Wed 15:00 P2/3OG

Hard-core bosonic dynamical mean-field study on melting of excitonic dispersion in $LaCoO_3$ — •Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1,3], Keisuke Tomiyasu[4], Davide Betto[5], Nicholas B. Brookes[5], Yohei Uemura[2], Mahnaz Ghiasi[2], Frank M. F. de Groot[2], and Jan Kuneš[1,6] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Debye Institute for Nanomaterials Science, Utrecht University, Universiteitsweg 99, 3584 CG Utrecht, The Netherlands — [3]Akhiezer Institute for Theoretical Physics, NSC KIPT, Akademichna 1, 61108 Kharkiv, Ukraine — [4]Department of Physics, Tohoku University, Aoba, Sendai 980-8578, Japan — [5]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, CS40220, F-38043 Grenoble Cedex 9, France — [6]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We study excitonic nature of the spin-state transition in $LaCoO_3$. Based on Co L_3-edge resonant inelastic x-ray scattering (RIXS) data, we construct an effective bosonic model which describes (i) intermediate-spin (S=1, IS) excitons propagating on a low-spin (S=0) background and (ii) a high-spin (S=2, HS) state as tightly-bound two IS excitons. The effective model is solved at finite temperatures by means of hard-core bosonic dynamical mean-field theory (HB-DMFT). The RIXS data across the spin-state transition around 100K reveals melting of the IS excitonic dispersion. The HB-DMFT analysis of the RIXS data points out a novel picture of the HS state as bi-exciton dressed by virtual fluctuations HS↔IS+IS.

TT 47.16 Wed 15:00 P2/3OG

Electronic properties of strongly correlated ruthenates — •Neda Riahisamani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425, Germany

We study the electronic properties of strongly correlated ruthenates by using the LDA+DMFT method. We construct materials-specific models for the t_{2g} bands via maximally localized Wannier functions. We solve the DMFT quantum impurity problem adopting as solver the weak coupling continuous-time Quantum Monte Carlo approach, in the implementation of Refs. [1, 2, 3]. Results will be discussed.

[1] E. Gorelov, M. Karolak, T. O. Wehling, F. Lechermann, A. I. Lichtenstein, E. Pavarini, Phys. Rev. Lett. **104**, 226401 (2010)
[2] G. Zhang, E. Gorelov, E. Sarvestani, E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)
[3] E. Sarvestani, G. Zhang, E. Gorelov, E. Pavarini, Phys. Rev. B **97**, 085141 (2018)

TT 47.17 Wed 15:00 P2/3OG

Response functions for correlated systems with LDA+DMFT — •Julian Musshoff[1,2] and Eva Pavarini[1,3] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]JARA-HPC, RWTH Aachen University, Aachen, Germany

Response functions are essential to compare theoretical calculations with experiments. For strongly correlated systems the calculation of the associated two-particle Green functions remains challenging, however. The state-of-the-art approach is the LDA+DMFT method. Here we adopt this technique; we use the strong-coupling continuous-time quantum Monte Carlo approach as the quantum impurity solver. Our massively-parallel general implementation [1,2] allows us to calculate response functions in different efficient polynomial bases. We will present recent results on the magnetic and orbital ordering mechanism in K_2CuF_4 [2]. In addition, we will discuss the application to layered cuprates, with and without doping.

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, *Phys. Rev. B* **87**, (2013) 195141
[2] J. Musshoff, G. Zhang, E. Koch, E. Pavarini, *Phys. Rev. B* **100**, (2019) 045116

TT 47.18 Wed 15:00 P2/3OG

Generic phase diagram of quantum dimer model on square lattice — Zheng Yan[1,2], •Zheng Zhou[1], Olav Syljuasen[3], Junhao Zhang[1], Tianzhong Yuan[1], Jie Lou[1,4], and Yan Chen[1,4] — [1]Department of Physics and State Key Laboratory of Surface Physics, Fudan University, Shanghai 200438, China — [2]Department of Physics, The University of Hong Kong, Hong Kong, China — [3]Department of Physics, University of Oslo, P. O. Box 1048 Blindern, N-0316 Oslo, Norway — [4]Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China

Constraint is an important property in low-energy physics, but it also bring a lot of difficulties for numeric calculation. The quantum dimer model is a low-energy description of many spin models, but its phase diagram is still controversial, even on the square lattice. In this article, we focus on the square lattice quantum dimer model and give a unified conclusion about its phase diagram which reconciles conflicting results given in the literature. With our newly developed sweeping cluster method, we studied the phase diagram of the almost full parameter space by introducing the definition of pair correlation function and other supporting evidence to distinguish the mixed phase from the columnar phase with high precision. In particular, we find that the ground state corresponds to the mixed phase for a vast parameter region.

TT 47.19 Wed 15:00 P2/3OG

Artificial Neural Networks Ansatz for Quantum Integrable Models — •Dennis Wagner[1,2], Andreas Klümper[1], and Jesko Sirker[2] — [1]Begische Universität Wuppertal — [2]University of Manitoba

Computing wave functions of quantum many-body systems is in general an exponentially hard problem. However, wave functions are required to calculate correlation functions. To approximate these wave functions, Artificial Neural Networks (ANN) have been considered.

In our work we investigate why this specific wave function ansatz seems to be useful for certain integrable models and how it can be improved. Furthermore, we try to get a deeper insight into quasi-local charges and compute dynamic correlation functions effectively.

TT 47.20 Wed 15:00 P2/3OG

Higher order auxiliary field quantum Monte Carlo methods — •Florian Goth and Fakher Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

The auxiliary field method QMC method has been a workhorse of solid state physics for a long time and has found its most recent implementation in the ALF package. The utilization of the Trotter-Suzuki decomposition to decouple the interaction from the non-interacting Hamiltonian makes this method inherently second order in terms of the imaginary time slice. We show the necessary generalizations to enable higher orders in ALF and perform numerical comparisons with other second order methods as well as methods of higher order.

TT 47.21 Wed 15:00 P2/3OG

Orbital differentiation in Hund metals — •Fabian B. Kugler[1], Seung-Sup B. Lee[1], Manuel Zingl[2], Hugo U. R. Strand[2], Andreas Weichselbaum[3], Gabriel Kotliar[4], Antoine Georges[2], and Jan von Delft[1] — [1]Ludwig-Maximilians-Universität München,

Germany — [2]Flatiron Institute - Simons Foundation, USA — [3]Brookhaven National Laboratory, USA — [4]Rutgers University, USA

Orbital differentiation is a common theme in multi-orbital systems, yet a complete understanding of it is still missing. Here, we focus on three-orbital Hubbard models to describe the t_{2g} bands of materials such as ruthenates and iron-based superconductors, and provide results of unprecedented accuracy by using the numerical renormalization group as real-frequency impurity solver for dynamical mean-field theory. First, we consider a minimal model for orbital differentiation, where a crystal field shifts one orbital in energy, and describe the various phases with dynamic correlation functions. Upon approaching the orbital-selective Mott transition, we find a strongly suppressed spin-coherence scale and uncover the emergence of a singular Fermi liquid and interband doublon-holon excitations. Then, we apply our method to the paradigmatic material Sr_2RuO_4 in a real-materials framework. We illustrate distinctive Hund-metal features and provide theoretical evidence for a Fermi-liquid scale of about 25 Kelvin.

TT 47.22 Wed 15:00 P2/3OG

Energy Gap in Strongly Correlated Hubbard Clusters—Comparing Green Functions and DMRG — •Sönke Hese[1], Jan-Philip Joost[1], Niclas Schlünzen[1], Claudio Verdozzi[2], Peter Schmitteckert[3], and Michael Bonitz[1] — [1]CAU Kiel, Germany — [2]Lund University, Sweden — [3]HQS Quantum Simulations, Germany

The (Fermi–)Hubbard model is a key system in the theory of strongly correlated electrons in solids. While the exact solution of the Hubbard Hamiltonian is known to possess a spin-symmetric ground state, in the mean-field approximation magnetic instabilities can, for on-site interactions beyond a critical U_c, induce the spontaneous breaking of spin symmetry leading to stable spin-density waves [1]. Using a Green function approach with higher order corrections to the self-energy, namely second Born and GW, we observe a similar effect at considerably larger interactions. Further, we find that similar inhomogeneous solutions are also present in spin-restricted calculations. By comparing to exact DMRG data for the 1D chain we find that these symmetry-broken states produce reliable data for the spectral function including the size of the Mott gap.

[1] J.-P. Joost, A.-P. Jauho, M. Bonitz, Nano Letters (2019), DOI:10.1021/acs.nanolett.9b04075

TT 47.23 Wed 15:00 P2/3OG

Symmetric WDA — •Asbjorn Rasmussen[1,2], Jens Jorgen Mortensen[1], and Kristian Sommer Thygesen[1,2] — [1]Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [2]Center for Nanostructued Graphene, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The Weighted Density Approximation (WDA) is an approximation to the exchange-correlation (xc) energy functional originally developed by D. J. Singh et al. and was shown to work well for a number of materials. WDA involves an approximation to the xc-hole that preserves the correct normalization, however the resulting pair-distribution is not symmetric. We expect that using a version of WDA that obeys the exact symmetry of the pair-distribution will generally improve results. In this work we implement a symmetric WDA using numerical techniques developed in the context of vdW functionals to calculate the non-local expressions efficiently.

TT 47.24 Wed 15:00 P2/3OG

Efficient ladder dual fermion calculations from a three-leg vertex — •Viktor Harkov[1,2], Angelo Valli[3], Alexander I. Lichtenstein[1], and Friedrich Krien[4] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]European X-Ray Free-Electron Laser Facility, 22869 Schenefeld, Germany — [3]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [4]Institut Jožef Stefan, Ljubljana, Slovenia

The calculation of the dynamical susceptibility within the dynamical mean-field theory requires the numerically expensive measurement of the vertex function of the auxiliary Anderson impurity model. We investigate an optimal parametrization of the vertex in terms of single-boson exchange (SBE). The approximation lowers the cost of ladder dual fermion calculations to a level comparable with the TRILEX approach.

TT 47.25 Wed 15:00 P2/3OG

The Chebyshev expansion as solver for the variational cluster approximation at finite temperature — •Jan Lotze and Maria Daghofer — University of Stuttgart, Functional Matter and Quantum Technologies, Pfaffenwaldring 57, 70569 Stuttgart

The variational cluster approximation (VCA) based on self-energy functional theory (SFT) [1] can be used to study correlated-electron Hamiltonians: Instead of the original systems self-energy, that of a 'reference system' is considered. While full diagonalisation suffices for small reference systems, larger systems require the Lanczos method or a quantum Monte Carlo method to be tractable. An alternative approach is to expand the reference systems Green's function in Chebyshev polynomials [2].

Here, thermodynamic and dynamical properties of the one- and two-dimensional Hubbard model at finite temperature are presented to illustrate the Chebyshev expansion in comparison to the Lanczos method as solver of the reference system.

[1] M. Potthoff, 'Self-Energy-Functional Theory', in Strongly Correlated Systems - Theoretical Methods (Springer, 2012)
[2] A. Braun and Schmitteckert, Phys. Rev. B **90**, 165112 (2014)

TT 47.26 Wed 15:00 P2/3OG

Magneto transport in light tuned STO-based interfaces — •Roland Schäfer, Daniel Arnold, and Dirk Fuchs — Institut fürFestkörperphysik, KIT, Karlsruhe

Recently we have shown that light can be utilized to tune transport properties of strontium titanate based interfaces at low temperatures in a controlled manner [1]. The effect has been observed at the interface with lanthanum aluminate and aluminum oxide. Light exposure at temperatures below $T = 1\,\mathrm{K}$ leads to a persistent reduction of resistance. The reduction depends on exposure dose, can be as large as a factor of five, and is accompanied by a reduction of the superconducting transition temperature reminiscent of the overdoped side of the dome structure in back gate experiments. Persistent changes can be reverted by heating the samples to a moderate temperature of about $T \approx 15\,\mathrm{K}$.

Here we present and discuss magneto transport data. The well established band structure of the two dimensional electron gas at the surface is used to calculate the conductance tensor as function of the magnetic field by semiclassical transport theory. The theoretical results are compared to the experimental findings.

[1] D. Arnold et. al, APL **115**, 122601 (2019)

TT 47.27 Wed 15:00 P2/3OG

RKKY driven quenching of local moments in Kondo dominated multi impurity models and Kondo insulators — •Fabian Eickhoff and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, Dortmund

For a single spin $\vec{S}$ ferromagnetically coupled to a metallic host, the Kondo effect is absent and a spinful groundstate remains. However, if an additional Anderson-type impurity orbital O is added, such that antiferromagnetic RKKY interaction $J_{\mathrm{RKKY}}\vec{S}_O\vec{S}$ is generated, $\vec{S}$ will always be quenched at zero temperature. For $T_{\mathrm{K}}^O \gg J_{\mathrm{RKKY}}$, the quenching occurs below the temperature scale $\tilde{T} \propto \exp(-T_{\mathrm{K}}^O/J_{\mathrm{RKKY}})$ where $\langle\vec{S}_O\vec{S}\rangle \approx 0$ at all temperatures. Using a new type of approximation for the wide band limit, we demonstrate that such a RKKY driven quenching of local moments on a scale $\tilde{T}$ occurs in multi impurity Anderson Hamiltonians as well, requiring at least three impurity sites. We show, that the formation of local moments due to a single Kondo-hole, is a direct consequence of RKKY driven local moment quenching and associated with an exponentially suppressed $\tilde{T}$. This goes beyond the scope of well established two impurity physics and sheds some new light on emerging magnetic moments and their screening in multi-impurity models as well as in periodic systems.

TT 47.28 Wed 15:00 P2/3OG

Dynamical Effects in Topological Kondo Insulators — •Marvin Lenk and Johann Kroha — Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany

Topological Kondo insulators (TKIs) are a new class of topological insulators, emerging through the interplay of strong correlations and spin-orbit coupling [1]. In TKIs, the bulk is a narrow band insulator due to the appearance of a localized Kondo resonance near the Fermi level and its hybridization with the conduction band. Additionally, the strong spin-orbit coupling of the localized moments generates a non-local hybridization between the local moments and the conduc-

tion band, which results in a topologically nontrivial band structure and gapless surface states.

In the past, TKIs have been described predominantly by slave-boson mean-field (SBMF) calculations. Such static methods are unable to capture finite life-time effects of the heavy Kondo quasiparticles. It is therefore not possible to investigate physics at the boundaries, like the dynamical emergence of topological edge states, where SBMF calculations become uncontrolled. We design a spin-orbit coupled dynamical mean-field theory (cf. [2]) with an auxiliary-particle conserving approximation (cf. [3]) as an impurity solver. With this, we aim at calculating characteristic, observable quantities, like the surface conductivity, including life-time effects.

[1] M. Dzero et al., Phys. Rev. Lett. 104 (2010) 106408
[2] A. Georges, AIP Conference Proceedings 715, 3 (2004)
[3] J. Kroha and P. Wölfle, Acta Phys. Pol. 29 (12), 3781 (1998)

TT 47.29 Wed 15:00 P2/3OG

Electronic and magnetic properties of Co impurity in Cu Host — •Daria Medvedeva[1], Alexander Poteryaev[2], Jindřich Kolorenč[1], and Alexander Shick[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Institute of Metal Physics of the Russian Academy of Sciences, Yekaterinburg, Russian Federation

The electron correlations play a crucial role in understanding of quantum matter. The Kondo effect that originates from scattering of itinerant electrons by local moments and corresponding screening is a manifestation of these many-electron correlations. Realistic multi-orbital approaches have to be applied in order to explain the experimental properties of Kondo 3*d* impurities in the bulk [1] and at the surface [2]. We consider the solution of multi-orbital single impurity Anderson model (SIAM) making use of CT-QMC (CT-HYB) and Exact diagonalization (ED based on Lanczos) for the Co impurity in bulk Cu. The model is parametrized using LDA computed hybridization function, and the crystal field. Spectral functions calculated by the ED method are in good agreement with QMC. It is found that the ground state of the impurity model is a singlet for different occupations of the impurity *d*-shell, that is, the Co magnetic moment is screened by Cu conduction electrons.

[1] L. Joly et al. Phys. Rev. B 95, 041108(R) (2017)
[2] R. Mozara et al., Phys. Rev. B 97, 085133 (2018)

TT 47.30 Wed 15:00 P2/3OG

Restoring the continuum limit in the time-dependent numerical renormalization group approach — •Jan Böker and Frithjof Anders — TU Dortmund, Theoretische Physik II, Otto-Hahn-Straße 4, 44227 Dortmund

We analytically construct a set of additional reservoirs coupled to the Wilson chain to recover the original continuous coupling functions to a quantum impurity.

We present a hybrid time-dependent numerical renormalization group (TD-NRG) approach which combines an accurate NRG treatment of the non-equilibrium dynamics on the finite size Wilson chain with a Bloch-Redfield formalism to include the effect of the additional reservoirs. For the solution of the Lindblad-style master equations a Lanczos method is employed. Our proposed approach tackles the intrinsic shortcoming of the TD-NRG induced by the bath discretization with a Wilson parameter $\Lambda > 1$. The effects of conservation laws and charge reflections along the Wilson chain are damped due to dissipation into the reservoirs, and a correct thermalization even on longer timescales is reached. The presented hybrid TD-NRG approach is used to investigate the real-time nonequilibrium dynamics in fermionic quantum-impurity systems. An analytical solution of the resonant-level model (RLM) serves as a benchmark for the accuracy of the method which is then applied to non-trivial models, such as the interacting RLM and the single impurity Anderson model.