# TT 20: Poster Session: Correlated Electrons 2

Time: Monday 15:00–19:00 Location: P2-OG1

TT 20.1 Mon 15:00 P2-OG1

**Mott-Hubbard transition in the mass-imbalanced Hubbard model** — •Marie-Therese Philipp, Markus Wallerberger, Patrik Gunacker, and Karsten Held — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

The mass-imbalanced Hubbard model (HM) represents a continuous evolution from the Hubbard to the Falicov-Kimball model. We employ DMFT and study the paramagnetic metal-insulator transition (MIT). Our results indicate that the MIT rather resembles that of the HM as soon as a tiny hopping between the more localized fermions is switched on. Further due to the equalising power of the Kondo e ect, the MIT occurs simultaneously for both spin species, opposed to what is known for the multi-orbital HM.

TT 20.2 Mon 15:00 P2-OG1

**LDA+DMFT approach to core-level X-ray spectroscopy for transition metal compound** — •Atsushi Hariki[1], Takayuki Uozumi[2], and Jan Kuneš[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Department of Mathematical Sciences, Graduate School of Engineering, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan

We perform systematic theoretical analysis of $2p$ core-level X-ray photoemission spectroscopy (XPS) of transition-metal compounds by means of the LDA+DMFT-based theoretical framework, which was recently developed [1,2]. In recent high-resolution and bulk-sensitive experiments, fine spectral features have become observed in the main-line (ML) structure of the $2p$ XPS. An account for these spectral features is essentially beyond the capability of theoretical models, such as the cluster model, conventionally employed in the analysis of $2p$ XPS. We reproduce the ML features by the new framework and show that these fine spectral features provide rich information on valence states including spin and orbital orderings.

[1] A. Hariki et al., J. Phys. Soc. Jpn. 82, 043710 (2013).
[2] A. Hariki et al., Eur. Phys. Lett. 114, 27003 (2016).

TT 20.3 Mon 15:00 P2-OG1

**Systematic analysis of Lock-Crisp-West (LCW) back-folding** — •Markus Dutschke[1], Michael Sekania[1,2], and Liviu Chioncel[1,3] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Andronikashvili Institute of Physics, Tamarashvili 6, 0177 Tbilisi, Georgia — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

The LCW theorem provides a analytic transformation of the momentum distribution, obtained either by Compton profile or positron angular correlation measurements, into the electronic distribution in the irreducible part of the Brillouin zone. It is typically employed to identify Fermi surface sheets as discontinuities of the obtained data for the system under consideration. In practice, however, the measured or computed projected momentum distributions are of finite precision and limited in momentum range. These restrictions introduce artificial discontinuities in the LCW back-folded data, resulting in unphysical Fermi surface features. In our study we present a systematic analysis of different practical LCW implementations, which reduce artifacts of the transformation and increase accuracy. We present results for elemental bcc and fcc metals with already well known Fermi surfaces.

TT 20.4 Mon 15:00 P2-OG1

**Characterization of the Mott-insulating phase in the one-dimensional fermionic Hubbard model** — •Daniel Duarte, Daniela Pfannkuche, and Marta Prada — I. Institut für Theoretische Physik, Universität Hamburg

In general, many-body long range correlations after a localized quench show non-trivial behavior. We focus on the one dimensional Hubbard model in the Mott-insulating phase and we investigate the evolution of the characteristic long range correlations. The spatial dependence of the correlation functions on the interaction strength is investigated at low temperatures. Furthermore, the spatial-temporal spread of the correlations after a sudden localized perturbation is calculated within a many-body description. Our analysis is based on a density matrix renormalization group approximation.

TT 20.5 Mon 15:00 P2-OG1

**Field Control of Magnonic Heat Flow** — •Benjamin Köhler and Wolfram Brenig — Institute for Theoretical Physics, Technische Universität Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Controlling such transport by means of external fields is vital for potential device design. Here we study thermal conductivity of a two dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of either external magnetic or electric fields. These fields are used to manipulated the heat flow, due to spin canting for the former and due to coupling to an additional Dzyaloshinsky-Moriya interaction for the latter. Using nonlinear spin wave theory and a Kubo approach we evaluate the thermal conductivity taking into account current relaxation by extrinsic mechanisms, as well as intrinsic magnon decay for finite magnetic fields. Semi-quantitative estimates for attainable variations of the heat conductivity in realistic materials will be presented as a function of the temperature and the external fields.

TT 20.6 Mon 15:00 P2-OG1

**Stochastic analytic continuation of Quantum Monte Carlo data** — •Niklas Casper and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Analytical continuation of imaginary time data from Quantum Monte Carlo methods is a notoriously complicated numerical task which is mathematically ill posed. Recently, stochastic analytic continuation (SAC) methods, which map the inversion from imaginary time to real frequencies onto a classical field theory at a fictitious temperature, have been introduced as a potential superset of conventional maximum entropy methods (MEM). We provide a complementary analysis of spectra obtained from SAC as well as MEM, resulting from various test models, as well the dynamic structure factor of a prototypical spin chain. We analyze the thermodynamics of the SAC considering various proposals for the choice of an optimal fictitious temperature. Moreover, we implement an auxiliary parallel Wang-Landau algorithm to provide for an unbiased determination of the spectrum, using the prior probability.

TT 20.7 Mon 15:00 P2-OG1

**Reduced Density-Matrix Functionals from Green's Functions** — •Heike Eisenlohr[1], Ebad Kamil[1], Robert Schade[2], and Peter Blöchl[2] — [1]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany — [2]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany

A new method for the electronic structure calculations of strongly correlated materials is explored. The long-term goal is the efficient simulation of such materials in the context of first-principles calculations. The method rests on an exact theorem, which expresses the one-particle reduced density-matrix functional by many-particle Green's functions via the Luttinger-Ward functional [1]. This theorem makes contact between ground state approaches such as reduced density matrix functional theory (rDMFT) and Feynman diagrams and even non-perturbative many-particle methods. The theorem suggests new approximate methods for the construction of density matrix functionals, namely to first establish an empirical Green's function as a direct function of the reduced density matrix, and secondly to evaluate the energy for this Green's function with many-particle methods. We present results based on a diagrammatic expansion and discuss difficulties and successes on the example of the Hubbard dimer.

This work is supported by the Deutsche Forschungsgemeinschaft via FOR1346 through project P9.

[1] P. E. Blöchl et al., Phys. Rev. B 88, 205139 (2013).

TT 20.8 Mon 15:00 P2-OG1

**From local to non-local correlations: the Dual Boson perspective** — •Arthur Huber — Universitaet Hamburg

Extended dynamical mean-field theory (EDMFT) is insufficient to describe non-local effects in strongly correlated systems, since corrections to the mean-field solution are generally large. We present an efficient scheme for the construction of diagrammatic extensions of EDMFT that avoids usual double counting problem by using an exact change of variables (the dual boson formalism) to distinguish the correlations

included in the mean-field solution and those beyond. With a computational efficiency comparable to EDMFT+GW approach, our scheme significantly improves on the charge order transition phase boundary in the extended Hubbard model.

TT 20.9 Mon 15:00 P2-OG1

**Susceptibility calculations using a multi-orbital general CT-QMC solver for DMFT** — •Julian Musshoff[1,2], Amin Kiani[1], and Eva Pavarini[1] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, 52425 Juelich, Germany — [2]Institute for Theory of Statistical Physics RWTH Aachen University, 52074 Aachen, Germany

Susceptibilities describe the response of a system to an external perturbation, and are therefore essential to compare theoretical calculations with experiments. We use a general continuous-time quantum Monte Carlo solver [1] for dynamical mean-field theory to calculate generalized local susceptibilities. Our general solver allows us to study multi-orbital correlated systems of any symmetry. We calculate the lattice susceptibilities using the Bethe-Salpeter equation. On the poster we show magnetic susceptibility results for a representative multi-orbital system, $KCuF_3$.

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, *Phys. Rev. B 87*, 195141

TT 20.10 Mon 15:00 P2-OG1

**Luttinger theorem in strongly correlated multi-orbital systems** — •Johannes Mitscherling[1,2] and Eva Pavarini[1] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

The Luttinger theorem stating that the volume enclosed by the Fermi surface is entirely determined by the total particle number was originally derived for a Fermi liquid in the zero temperature limit. We discuss the possible extension of the theorem for certain classes of strongly correlated systems outside the Fermi-liquid regime.

Similarly to Luttinger's sum rule, we present a sum rule for correlated multi-orbital systems at finite temperature. We identify an exact relation between the Fermi volume of a given band index and its occupation. This relation involves additional contributions which come into play in this generalized setting while they vanish for a Fermi liquid in the zero temperature limit. The study of these contributions enables us to identify conditions under which the Luttinger theorem is valid beyond its traditional scope.

As a first application, we apply the extended Luttinger sum rule to the two-site Hubbard model. As a second step, the extended Luttinger theorem is used to study the temperature evolution of the three Fermi sheets of $Sr_2RuO_4$.

TT 20.11 Mon 15:00 P2-OG1

**Screened Coulomb interaction for strongly correlated molecular crystals** — •Michael M. E. Baumgärtel and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

For strongly correlated molecular crystals we determine screened Coulomb Hubbard-parameters. The unscreened Coulomb interaction of correlated molecular orbitals (MOs) can directly be obtained from Hartree-integrals. This interaction is screened by the electrons in the uncorrelated MOs as these are polarized. We compute the screening due to the self-consistent electric fields arising from the induced distributed dipoles. To treat the polarized crystal, we develop an optimized Ewald summation of the Fourier-transformed dipole-dipole interaction. Employed on a Brillouin zone grid our method yields the screened inter-molecular Coulomb interaction for any charging pattern of the correlated MOs. The optimization of the convergence and performance of our method is demonstrated.

We present the screened Coulomb interaction e.g. for Fullerene crystals and discuss the accuracy and reliability of the results. While in the past only approximations of MOs as a single point-dipole where feasible, we discuss the effect of spacially extended MOs: For example for Fullerenes we approach the limit of point-dipoles by virtually shrinking the Fullerene radius and we determine the renormalization of the polarizabilities due to distribution of the MOs.

TT 20.12 Mon 15:00 P2-OG1

**Scaling Behavior of the Compton Profile of Alkali Metal Elements** — •Michael Sekania[1,2], Wilhelm Hans Appelt[3,4], Diana Benea[5], Hubert Ebert[6], Dieter Vollhardt[1], and Liviu Chioncel[1,4] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Andronikashvili Institute of Physics, 0177 Tbilisi, Georgia — [3]Theoretical Physics II, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [5]Faculty of Physics, Babes-Bolyai University, Ro-400084 Cluj-Napoca, Romania — [6]Department of Chemistry, University Munich, D-81377 München, Germany

The contribution of the valence electrons to the Compton profiles of the alkali metals is calculated using density functional theory. We show that the Compton profiles can be modeled by a $q-$Gaussian distribution, which is characterized by an anisotropic, element dependent parameter $q$. Thereby we derive an unexpected scaling behavior of the Compton profiles of all alkali metals.

TT 20.13 Mon 15:00 P2-OG1

**Exact Diagonalization study of large Hubbard clusters** — •Michael Danilov[1], Sergei Iskakov[2], Malte Harland[1], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik Jungiusstrasse 9, 20355 Hamburg, Germany — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA

Using efficient exact diagonalization scheme, we studied electronic structure of 4x4 doped Hubbard cluster with realistic hopping parameters including next nearest neighbour hopping t′ = -0.3t, which is optimal for superconducting cuprates. The Green's function and abnormally large density of states near Fermi level are analysed as function of doping and strength of local Coulomb interactions.

In order to compare the spectrum of the 16-site cluster against small 2x2 plaquette, where the ground state is 6-fold degenerate for special values of Coulomb interactions and chemical potential (Phys. Rev. B 94 (2016) 125133), we scale the hopping between the 4 plaquettes constituting the cluster with auxiliary parameter $\alpha$.

We examined the degeneracy of low-energy spectra as function of $\alpha$ and local Coulomb interaction U and visualised the ground state wavefunction. Our current standpoint is that the optimal Coulomb interaction is close to U=10t, versus U=6t for degenerate ground state of isolated plaquette. We discuss the relevance of degenerate low-energy spectra with regard to possible mechanism of the high-temperature superconductivity.

TT 20.14 Mon 15:00 P2-OG1

**Quantum-Many-Body Intermetallics: Phase Stability of Fe 3 Al and Small-Gap Formation in Fe 2 VAl** — •Oleg Kristanovski — I. Institut für Theoretische Physik Jungiusstrasse 9, 20355 Hamburg, Germany

Various intermetallic compounds harbor subtle electronic correlation effects. To elucidate this fact for the Fe-Al system, we perform a realistic many-body investigation based on the combination of density functional theory with dynamical mean-field theory in a charge self-consistent manner. A better characterization and understanding of the phase stability of bcc-based D0 3 -Fe 3 Al through an improved description of the correlated charge density and the magnetic-energy is achevied. Upon replacement of one Fe sublattice by V, the Heusler compound Fe 2 VAl is realized, known to display bad-metal behavior and increased specific heat. We here document a charge-gap opening at low tem- peratures in line with previous experimental work. The gap structure does not match conventional band theory and is reminiscent of (pseudo)gap charateristics in correlated oxides.

TT 20.15 Mon 15:00 P2-OG1

**Reservoir-induced Collapse and Revival of Photon BEC Oscillations** — •Bastian Havers, Tim Lappe, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

A true photon Bose-Einstein condensate (BEC) was first realized in 2010 [1] by filling a dense photon gas into a dye-filled, optical microcavity by means of a laser and subsequently thermalizing it at room temperature. Most recently, the dynamics is being investigated by means of Josephson oscillations of the photon BEC in double-well potential traps. It is characterized by a collapse and revival of Josephson oscillations. We develop the theory for the photon BEC dynamics, coupled to the dye. The ensemble of dye molecules is described as a structured, dissipative bath of three-level systems, involving three different processes, photon absorption with absorption rate $1/\tau_a$, dark transitions, and photon re-emission with emission rate $1/\tau_e$. The BEC dynamics is treated on the Gross-Pitaevskii level in a two-mode ap-

proximation for the BECs in the two potential wells [2].

[1] J. Klaers, J. Schmitt, F. Vewinger, and M. Weitz, Nature **468**, 545 (2010).
[2] A. Smerzi, S. Fantoni, S. Giovanazzi, and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997)

TT 20.16 Mon 15:00 P2-OG1

**Higher-order local and non-local correlations for 1D strongly interacting Bose gas** — EJKP Nandani[1,2,3], •Rudolf A Römer[4], Shina Tan[5,6], and Xi-Wen Guan[1,7] — [1]Wuhan Institute of Physics and Mathematics, CAS, Wuhan 430071, China — [2]Chinese Academy of Sciences, Beijing, China — [3]University of Ruhuna, Matara, Sri Lanka — [4]University of Warwick, Coventry CV4 7AL, UK — [5]Georgia Institute of Technology, Atlanta, GA, USA — [6]Center for Cold Atom Physics, Wuhan, China — [7]Australian National University, Canberra ACT 0200, AUS

The correlation function is an important quantity in the physics of ultracold quantum gases because it provides information about the quantum many-body wave function beyond the simple density profile. In this paper we first study the $M$-body local correlation functions of the one-dimensional (1D) strongly repulsive Bose gas within the Lieb-Liniger model using the analytical method proposed by Gangardt and Shlyapnikov (2003 Phys. Rev. Lett. 90 010401; 2003 New J. Phys. 5 79). In the strong repulsion regime the 1D Bose gas at low temperatures is equivalent to a gas of ideal particles obeying the non-mutual generalized exclusion statistics with a statistical parameter $\alpha = 1 - 2/\gamma$. Here $\gamma$ is the dimensionless interaction strength within the Lieb-Liniger model. We rigorously prove that such a statistical parameter solely determines the sub-leading order contribution to the $M$-body local correlation function of the gas at strong but finite interaction strengths. We explicitly calculate the correlation functions at zero, low, and intermediate temperatures.

TT 20.17 Mon 15:00 P2-OG1

**Spin dynamics in classical XXZ chains with disorder** — •Tim Dierker and Robin Steinigeweg — University Osnabrück

The transport of magnetization is analyzed for the classical XXZ spin chain with a random magnetic field. In order to do so, the Hamiltonian equations of motion are solved numerically for initial states realizing harmonic-like magnetization profiles with small amplitudes and with random phases. Without disorder, the resulting dynamics are observed to be diffusve in a hydrodynamic regime starting at comparativley small times and wave lengths [1]. The influence of disorder on these dynamics is studied in the entire range from weak to strong disorders.

[1] R. Steinigeweg, Europhysics Letters 97, 67001 (2012)

TT 20.18 Mon 15:00 P2-OG1

**Numerical Study of the Kitaev-Heisenberg Chain** — •Cliò Efthimia Agrapidis[1,2], Jeroen van den Brink[1,2], and Satoshi Nishimoto[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Department of Physics, Technical University Dresden, 01069 Dresden, Germany

In recent years, because of the emergence of candidate materials and the interest in the spin liquid state realization, there has been a growing number of studies on the Kitaev model, at first, and on the Kitaev-Heisenberg (KH) after. Adding the Heisenberg-type interaction to the initial, exactly integrable, model is necessary and inevitable for any realistic description. Nevertheless, the vast majority of these studies is focused on 2-dimensional lattices (honeycomb, triangular), while research on the KH chain is lacking.

Motivated by this, we study the KH chain using the exact diagonalization and the density matrix renormalization group techniques. We present the phase diagram as a function of an angle parameter $\phi$, setting the Heisenberg interaction to $\cos\phi$ and the Kitaev one to $\sin\phi$. We identify five different possible phases; namely, Heisenberg, incommensurate, ferromagnetic, XY and Néel phases, by calculating total spin, central charge, static structure factor, and the Néel and XY order parameters. Moreover, we investigate specific features of the dynamical structure factor in each phase. In addition, we present some of the above calculations in the presence of an applied magnetic field.

TT 20.19 Mon 15:00 P2-OG1

**Topological properties of classical spin spirals from an exact mapping to free fermions** — •Jan Attig and Simon Trebst — University of Cologne

In classical magnets coplanar spin spirals often arise in the presence of competing interactions which suppress more conventional types of magnetic order. Here we demonstrate that the physics of these coplanar spin spirals can be understood from an exact mapping of the classical Heisenberg model on a geometrically frustrated lattice to a free-fermion model on a closely related "squared" lattice. This one-to-one correspondence not only allows to make a connection between the Fermi surface of the free fermion model and the manifold of degenerate spiral states, but also allows to discuss topological phenomena of the free-fermion band structure in the corresponding classical magnet.

TT 20.20 Mon 15:00 P2-OG1

**Competing spin textures in j=1/2 Mott insulators on the triangular lattice** — •Tilman Disselkamp and Simon Trebst — University of Cologne

Similar to their well-studied electronic counterparts, quantum magnets exhibit a wealth of novel phenomena in the presence of strong spin-orbit coupling. Of particular interest are Kitaev materials, spin-orbit entangled j=1/2 Mott insulators where topology plays a key role in the formation of magnetic order – either in the emergence of spin liquid physics or, of interest here, the formation of non-trivial spin textures. Specifically, we consider j=1/2 Mott insulators in triangular lattice geometries, relevant e.g. to the sister compounds $Ba_3IrTi_2O_9$ and $Ba_3TiIr_2O_9$ for which we study the interplay of geometric frustration and spin-orbit coupling. The latter gives rise to Kitaev or Dzialoshinskii-Moriya interactions that stabilize a $Z_2$ vortex crystal or a skyrmion crystal, respectively. Using classical Monte Carlo simulations, we map out the stability and interplay of these spin textures in a magnetic field at zero and finite temperatures.

TT 20.21 Mon 15:00 P2-OG1

**Universal short-time response and formation of correlations after quantum quenches** — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Avenida Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The short-time evolution of two distinct systems, the pump and probe experiments with semiconductor and the sudden quench of cold atoms in an optical lattice, is found to be described by the same universal response function. This analytic formula at short time scales is derived from the quantum kinetic theory approach observing that correlations need certain time to be formed. The influence of a finite trapping potential is derived and discussed as well as Singwi-Sjølander local field corrections. The quantum kinetic equation allows to understand how two-particle correlations are formed and how the screening and collective modes are build up.

[1] K. Morawetz, Phys. Rev. B 90 (2014) 075303
[2] K. Morawetz, Phys. Rev. E 66 (2002) 022103
[3] K. Morawetz, M. Bonitz, V. G. Morozov, G. Röpke, D. Kremp, Phys. Rev. E 63 (2001) 20102
[4] K. Morawetz, V. Spicka, P. Lipavský: Phys. Lett. A 246 (1998) 311